Positronic lithium, an electronically stable Li–e^+ ground state

G.G. Ryzhikh* and J. Mitroy

Faculty of Science, Northern Territory University, Darwin NT 0909, Australia

Abstract

Calculations of the positron-Li system were performed using the Stochastic Variational Method and yielded a minimum energy of −7.53208 Hartree for the $L = 0$ ground state. Unlike previous calculations of this system, the system was found to be stable against dissociation into the Ps + Li^+ channel with a binding energy of 0.00217 Hartree and is therefore electronically stable. This is the first instance of a rigorous calculation predicting that it is possible to combine a positron with a neutral atom and form an electronically stable bound state.

One of the most tantalizing questions of positron physics is whether it is possible for a positron to bind itself to a neutral atom and form an electronically stable state [1,2]. This is a question which can only be answered by a sophisticated calculation (or experimentation) as the mechanisms responsible for binding the positron to the atom are polarization potentials present in the positron-atom complex. The accurate computation of the polarization potential for a positron–atom (or electron–atom) system is of course a challenging exercise in many body physics.

While the question of whether it is possible to bind a positron to a neutral atom is an open question, the ability of positronium to attach itself to atoms has been known for a long time. A number of previous works have demonstrated that the positronium–hydride (PsH) species [3–8] is stable against dissociation into the Ps + H or the $e^+ + H^-$ channels. In this case, binding is more likely since the positron is binding itself to a species with an overall negative charge.

The question of whether a positron can form an electronically stable bound state with a neutral atom is more vexing. Dzuba et al [9] have made calculations suggesting that it is possible to bind a positron to atomic species with two valence electrons such as Mg, Zn, Cd and Hg. These calculations were performed in the framework of many–body perturbation theory and their results, while suggestive, cannot be regarded as providing proof to the existence to electronically stable positronic atoms.

In their work, Dzuba et al [9] did not consider the possibility of positrons forming bound states with alkali atoms such as Li, Na, K, ... even though the polarization potential for these species should be stronger than for the alkaline and alkaline earth atoms and therefore the possibility of binding should be improved. One difficulty in binding positrons to alkali atoms is that the ionization energy of the alkali atoms is smaller than the binding energy of positronium. Therefore the binding energy of the positron to the neutral atom must exceed a particular value for the species to be stable against dissociation into positronium + ion. For example, for the Li–e^+ species to be stable against dissociation into positronium plus Li^+ requires that the binding energy of the e^+ with respect to the Li ground state be greater

than $(0.25-0.19815)$ Hartree. In this respect, it is more appropriate to regard the possibility of binding as a question of whether Ps can itself bind to Li^+.

Previous works [5,10] on this species had shown that while the Li–e^+ system can have a total energy lower than neutral Li, the energy was not low enough to prevent dissociation into Ps + Li^+. In this work, a large variational calculation of the Li–e^+ system is performed using the Stochastic Variational Method of Varga and Suzuki [11]. In contradiction with previous works it is found that the ground state is electronically stable and the binding energy for this state is calculated.

A Gaussian basis has long been a popular tool for variational calculations in various areas of quantum physics and chemistry. The Gaussian basis used in this work has two very important features that make it possible to generate very accurate wave functions for few body systems. First, the matrix elements of the interaction Hamiltonian can be calculated analytically or, at worst, reduced to a one-dimensional integral for any number of particles. Second, that part of the wave function concerned with the spatial coordinates maintains its functional form after any possible permutation of the particles. This is a very useful property for studying systems containing identical particles.

The Stochastic Variational Method (SVM) was initially proposed as a method suitable for solving nuclear structure problems involving a small number of particles [12,13]. The main idea behind the method is to use stochastic techniques to optimize the non-linear parameters (i.e. the exponents) of the underlying Gaussian basis. Since the Gaussian basis contains terms with r_{ij}^2 correlation factors, the method is capable of achieving results of the highest accuracy provided the non-linear parameters are properly optimized.

In recent years, the SVM and related methods have been used by many groups to perform high precision variational calculations in atomic, mesoatomic, hypernuclear and multiquark systems [7,14–16]. Recently, the SVM has been modified to allow the calculation of excited states and also to permit the use of a wide variety of non-central forces [17,18]. In this work, the program of Varga and Suzuki [11] (which can be used with arbitrary pairwise central forces) was used for the calculations. A detailed description of the method and the results

of test calculations on various atomic and nuclear system containing 3–6 particles can be found in [11,17].

An initial series of calculations on a variety of related species were performed to estimate the uncertainties in the present calculation and validate the method. Results of our calculations for neutral Li, neutral Be, and the PsH species are shown in Table I and compared with other accurate nonrelativistic calculations. We show results that were computed with an infinite nuclear mass to simplify comparison with the other results in Table I. Our calculation for PsH, agreed with the best previous calculation to within 4×10^{-6} Hartree [7]. Results for the more complicated Be and Li^- species underestimate the best calculations [20] by less than 7.0×10^{-4} Hartree.

Since the question of whether an electronically stable bound state exists depends on the energy relative to the sum of the energies for the Li^+ and Ps atoms, the energy of the Li^+ ground state was computed. Our result is identical with that of the classic calculation of Pekeris [22] to 8 significant figures and indicates that binding will occur if the total energy of the Li-e^+ system is lower than -7.529913 Hartree.

The convergence of energy of the Li–e^+ system as a function of the number of gaussoid basis functions is shown in the Table II. It is noticeable that a very large calculation, including at least 300 gaussoid basis functions, was needed before definite evidence of a bound state was obtained. The largest calculation included 800 basis functions, and resulted in a total energy of $E = -7.53208$ Hartree which is equivalent to a binding energy of $\varepsilon = 0.00217$ Hartree. When reference is made to the binding energy of the Li–e^+ system it should be noted that the binding energy is relative to breakup into Li^+ and Ps.

Energy expectation values were also computed with the present optimized wave functions for a finite mass. The ^{7}Li nucleus has a mass of $M = 12863.2m_e$ and for this species we obtained $E(300) = -7.279325$ Hartree for Li^+, and $E(800) = -7.531491$ Hartree for Li–e^+ giving a binding energy of $\varepsilon = 0.00217$ Hartree. For most purposes, finite mass effects can be ignored since they will not change the binding energy by more than 1%.

The statement that a bound state exists also remains valid when relativistic effects are

taken into consideration. One estimate of the relativistic energy correction for neutral Li is 0.000011 Hartree [21]. An energy correction of this size cannot affect the primary conclusion, namely the existence of an Li–e^+ bound state, but might have to be taken into consideration if a really precise value of the binding energy is to be achieved. Nevertheless, we are confident in asserting that the Li–e^+ ground state is electronically stable against decay into both the Li–e^+ and Li^+–Ps channels.

While the state is electronically stable, it is not stable against electron-positron annihilation. The dominant decay process for electron-positron annihilation is into two γ–rays. Therefore the two-photon annihilation rate $\Gamma_{2\gamma}$ was computed using the general formula,

$$\Gamma_{2\gamma} = \pi n \alpha^4 c a_0^{-1} < \delta_{-+} > \approx \ 50.30874045 \times 10^9 \ n < \delta_{-+} > \mathrm{sec}^{-1}, \tag{1}$$

which is valid for a system containing n electrons and one positron [7]. In the above expression, δ_{-+} is the expectation value of electon-positron Dirac δ function

$$< \delta_{-+} >= \frac{< \Psi | \delta(\mathbf{r}_{e^-} - \mathbf{r}_{e^+}) | \Psi >}{< \Psi | \Psi >} \tag{2}$$

The annihilation rate for the Li–e^+ system was $\Gamma_{2\gamma} = 1.70 \times 10^9$ sec^{-1}. The annihilation rate for PsH has been computed as a consistency check and the value we obtain, $\Gamma_{2\gamma} = 2.45 \times 10^9$ sec^{-1}, is consistent with the best previous estimate [7], namely $\Gamma_{2\gamma} = 2.436 \times 10^9$ sec^{-1}.

Other recent studies of the positron–Li system [5,10] had shown that an electronically stable bound state did not exist. The failure to find a bound state can be attributed to the difficulty in performing a calculation on a system containing 4 active particles that had to be accurate to 10^{-3} Hartree. The most recent study [10] of the Li–e^+ system used the Diffusion quantum Monte Carlo method to predict an energy of -7.5203 ± 0.0048 Hartree which only just failed to indicate a stable bound state. This calculation, correctly predicted the binding energy of the e^+–H^- system (-0.7891 ± 0.0020 Hartree) but evidently the calculation of Li–e^+ system is more exacting.

The configuration-interaction-Hylleraas calculation (CI-Hy) of Li–e^+ system by Clary [5] was performed by adapting a method that had previously been very successful for atoms

[23] and gave an energy of -7.5094 Hartree. As a similar calculation by Clary [5] of the PsH system underestimated the energy by 0.0050 Hartree it is not unexpected that it failed to predict a stable Li–e^+ system. Given that the CI-Hy method [23] gave an energy for neutral Be (-14.6665 Hartree) which agrees with the best current estimate to within 0.0008 Hartree it is interesting to speculate on the reason for the slower convergence of the method for systems containing a positron. The resolution of this puzzle probably lies in the fact that the correlations between an electron and a positron are distinctly different than the correlations between two electrons. A system involving purely electrons has two implicit features that will act to diminish the importance of inter-electronic correlations. First of all, the Pauli principle acts to keep electrons with the same spin away from each other. Second, the electron-electron interaction also acts to keep electrons away from each other. However, neither of these effects is present if an electron is replaced by a positron. The interaction between an electron and a positron is attractive, and it easy to imagine a system with one valence electron like lithium evolving into a configuration consisting of a positronium atom orbiting around a positively charged $(1s)^2$ core.

This possibility was investigated by projecting the Li–e^+ ground state wave function onto a wave function containing the product of the ground state positronium wave function and the two electron wave function for Li^+. The normalization of the residual part of the projected wave function (essentially the wave function for the Ps center of mass) was found to be 0.93. Therefore, the best heuristic model of the Li–e^+ ground state would be to regard the system as a positronium atom weakly attached to, and orbiting around a Li^+ $(1s)^2$ core.

The present calculation represents the first rigorous calculation giving positive evidence that it is possible to combine a positron with a neutral atom and form an electronically stable system. Although, the best ab-initio estimate of the binding energy, 0.00217 Hartree is subject to uncertainties due to incomplete convergence of the Li–e^+ energy, the statement that the system is electronically stable will certainly remain valid under any possible refinements of the model.

Having shown that it is possible to combine a positron with neutral Li to form an

electronically stable bound state, an immediate question arises as to whether it is possible to join a positron to a more complicated alkali atom such as sodium and also form a bound state. The answer to this question cannot be obtained with a calculation identical to the present calculation, rather the present method would have to be refined to incorporate the physics of a closed shell core. The possible existence of additional positronic atoms is a topic that is worth further investigation.

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TABLES

TABLE I. Non-relativistic energies (in Hartree) of various atomic systems compared with previous accurate results. In these calculations the nuclear mass has been assumed to be infinite. The number in parentheses refers to the total dimension of the gaussoid basis.

System	E (SVM, this work)	E ("best" nonrelativistic)
Li^+	–7.2799133 (300)	–7.2799133[a]
PsH	–0.789183 (400)	–0.789179 [b]
Li	–7.478041 (400)	–7.4780603[c]
Be	–14.66676 (601)	–14.66732 [d]
$Li + e^-$	–7.50012 (600)	–7.50076 [d]
$Li + e^+$	–7.53208 (800)	–7.5203 [e]

[a] reference [22]

[b] reference [7]

[c] reference [19]

[d] reference [20]

[e] reference [10]

TABLE II. Convergence of the Li–e^+ energy (in Hartree) as a function of basis size. Last column shows the energy relative to the Li^+–Ps threshold at -7.529913 Hartree.

E	basis size	ε
–7.52360	200	not bound
–7.52773	300	not bound
–7.52897	350	not bound
–7.53002	400	0.00011
–7.53084	500	0.00093
–7.53135	600	0.00144
–7.53165	700	0.00174
–7.53208	800	0.00217

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* E-mail: g_ryjikh@banks.ntu.edu.au

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